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QUADRATURE VARIATIONS IN DISCRETE-ORDINATES CALCULATIONS

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SUMMARY

Techniques to reduce the computer time required to solve neutron transport problems that use the discrete-ordinates (S_n) approximation were studied. These techniques are based on obtaining preliminary neutron flux distributions with low-order angular or spatial quadrature and then incorporating the high-order detail required for the final calculation. Results indicate that such modifications to the standard application of the S_n method can significantly decrease problem execution times.

From those sample problems in which converged solution accuracy identical to that of the standard S_n method application was required, several conclusions may be drawn: (1) If more than one angular quadrature set is employed, requiring full convergence on the preliminary set increases running time. (2) For problems specifying lower order final angular quadratures ($\leq S_8$), the most efficient approach to final convergence is through the use of a single preliminary S_2 quadrature followed by partial convergence on the final quatrature. The partial convergence limits the number of inner iterations and assures that the fluxes are equally well converged in each group before entering the final calculation. (3) For problems requiring high-order final angular quadratures ($> S_8$), the greatest time reduction is observed when several intermediate quadrature sets are used successively to approach final convergence. (4) For problems requiring highly detailed spatial information, the time to final convergence is reduced when a relatively coarse mesh is used to represent the spatial and material configuration in the preliminary calculation.

INTRODUCTION

Recent advances in computer design make it possible to obtain numerical solutions to problems previously too large to process. However, the direct application of existing methods to these larger problems can require prohibitively large expenditures of computer time. One class of problem of which this is particularly true, due to the

iterative procedure involved, is the numerical solution of the Boltzmann transport equation using the S_n , or discrete ordinates method (ref. 1).

The solution of the stationary transport equation

$$\hat{\Omega} : \nabla \psi(\mathbf{E}, \vec{\rho}, \hat{\Omega}) + \sigma_{t}(\mathbf{E}, \vec{\rho}) \psi(\mathbf{E}, \vec{\rho}, \hat{\Omega}) = \mathbf{S}(\mathbf{E}, \vec{\rho}, \hat{\Omega})$$
 (1)

entails the determination of a particle flux distribution which is a function of energy E, position $\vec{\rho}$, and direction $\hat{\Omega}$ in terms of the total cross section σ_t and the source S. In the S_n method, this is accomplished by establishing a quadrature on the domain of each of these independent variables and, using an initial approximate distribution, iterating on each quadrature until a specified degree of convergence is attained. Several techniques for improving the efficiency of the method by using various scaling (ref. 2) and acceleration (ref. 3) procedures to force more rapid convergence on the flux distribution have been successfully applied. Alternate techniques for directly reducing the number of numerical calculations involved by varying the manner in which the quadratures are applied seem to have been less thoroughly investigated. Thus, existing applications of the S_n method are basically similar (ref. 4) in that they require a constant order of quadrature for each of the independent variables.

In obtaining a solution to the transport equation for a problem in which no prior information concerning the flux distribution is available, it is customary to use as a first approximation a distribution which is constant in the independent variables. The major portion of the numerical calculation is then devoted to obtaining successively more accurate approximations to the flux distribution. Since the time required to perform an iteration depends strongly on quadrature order and since the accuracy of the early iterations is low, use of the high quadrature orders required for the final solution does not appear warranted in the preliminary stages of the calculation. A more optimum procedure might be to vary the quadratures as a function of the progress of the calculation so as to obtain a reasonably accurate preliminary flux distribution more rapidly.

Although the flux distribution is a function of energy, position, and direction, the energy quadrature is effectively removed from the actual discrete ordinates calculation due to the group averaging methods normally used. The two remaining independent variables, direction and position, will be discussed separately.

The central feature of the S_n technique is the representation of the continuous angular distribution of the particle flux by a number of discrete intervals. If the direction unit vector $\hat{\Omega}$ is defined by the angles μ , η , and ξ , it may be written, in rectangular coordinates, as

$$\hat{\Omega}_{m} = \cos \mu \hat{\mathbf{i}} + \cos \eta \hat{\mathbf{j}} + \cos \xi \hat{\mathbf{k}}$$
 (2)

where m denotes the total angular dependence. The direction $\hat{\Omega}_{m}$ represents a point on the surface on a unit sphere and has an associated surface area w_{m} , which indicates the weight assigned to that direction. The range of integration over the unit vector is divided into a number of intervals M corresponding to the order of the quadrature, and the angular flux is assumed to be constant within each interval. The integral over the angle may now be replaced with a summation over the weighted intervals so that the group scalar flux φ_{g} is given by

$$\varphi_{\mathbf{g}}(\vec{\rho}) = \frac{1}{4\pi} \int_{\hat{\Omega}} \psi_{\mathbf{g}}(\vec{\rho}, \hat{\Omega}) d^{2}\hat{\Omega} = \sum_{\mathbf{m}=1}^{\mathbf{M}} w_{\mathbf{m}} \overline{\psi}_{\mathbf{g}, \overline{\mathbf{i}}, \overline{\mathbf{k}}, \overline{\mathbf{m}}}$$
(3)

where $\psi_{g,\overline{i},\overline{k},\overline{m}}$ represents the average flux in an interval for a given direction.

Since the calculation time increases rapidly with the number of discrete intervals employed, limiting this number of directions in the initial stages of the calculation should be a valid procedure. Historically, several variations in the standard S_n procedure have attempted to achieve this end by first obtaining a preliminary flux distribution for use in the main calculation. Thus, some S_n codes have contained an option for first performing a diffusion theory solution (ref. 5) for first performing one outer iteration using an S_2 quadrature (ref. 6) or for reducing the number of inner iterations in the initial outer iterations (ref. 7). There seems to be little or no published information on the effect of these procedures on accuracy and running time.

In the standard S_n treatment, the spatial dependence of the particle flux is approximated by superimposing a finite mesh on the configuration to be analyzed. While the mesh spacing in any one direction is arbitrary, no variation is permitted in that mesh in an orthogonal direction. For example, in rectangular coordinates, the mesh set up along the x-coordinate must be retained for all values of the y-coordinate.

In the discrete ordinates method, determination of the value of the central average angular fluxes $\overline{\psi}$ involves the use of a physical model to relate the angular fluxes at the mesh cell boundaries with the central flux. In the commonly used 'diamond' model

$$\overline{\psi}_{g,\overline{i},\overline{k},\overline{m}} = \frac{1}{2} \left[\psi_{g,i+1,\overline{k},\overline{m}} + \psi_{g,i,\overline{k},\overline{m}} \right]$$

$$= \frac{1}{2} \left[\psi_{g,\overline{i},k+1,\overline{m}} + \psi_{g,\overline{i},k,\overline{m}} \right]$$

$$= \frac{1}{2} \left[\psi_{g,\overline{i},\overline{k},m} + \psi_{g,\overline{i},\overline{k},m-1} \right]$$

$$(4)$$

where i and k represent mesh boundaries in orthogonal directions and m again denotes the angular dependence. Since all these angular fluxes must be calculated repeatedly in each interval, for each quadrature direction, as indicated in equation (3), it is obvious that any method of eliminating unnecessary spatial mesh intervals would also reduce calculation time.

The objective of this study was to determine the general feasibility of reducing computer time in discrete ordinates calculations. In particular, several modifications to the standard \mathbf{S}_n procedure, which relax the constant quadrature requirements, were investigated and their effect on accuracy and calculation time observed.

ANALYSIS AND RESULTS

For this study, the modifications made to present applications of the discrete ordinates method are restricted to relaxation of the constant quadrature requirements. The primary objective in allowing quadratures to vary during the calculation is to establish improved scalar flux distributions more rapidly. This is accomplished by performing preliminary calculations with lower order quadratures, and a concomitant smaller number of angular fluxes, and using the resulting scalar fluxes to enter the final calculation.

Removal of the energy dependence from equation (1) results in a set of integrodifferential equations coupled by a source term involving only the scalar fluxes. In the normal flow of the discrete ordinates calculation there are two major iterative procedures. The first, or inner iteration, consists of a determination of the angular fluxes for all discrete directions over the entire spatial mesh. This results, as indicated in equation (3), in a revised scalar flux distribution. The second, or outer iteration, involves calculation of the source terms coupling each equation and involves only these scalar fluxes. Since this outer iteration is essentially independent of the angular fluxes, the completion of each such iteration affords a convenient point at which to vary angular quadratures.

While it is also possible to vary the spatial mesh on termination of an outer iteration, modifications to the angular and spatial quadratures are not analogous. Permissible variations in the spatial mesh should comprise not only alterations in the order of the uniform mesh but, more importantly, the elimination or combination of noncritical mesh intervals. This latter consideration requires that some assumptions be made regarding the behavior of the individual angular fluxes.

Because of the dissimilar procedures involved, the modifications to the angular and spatial quadratures will be treated separately. All modifications were made utilizing an existing two-dimensional S_n program (ref. 3) TDSN. TDSN is a variable storage allocation code which is similar in flow diagram to other current discrete ordinates codes.

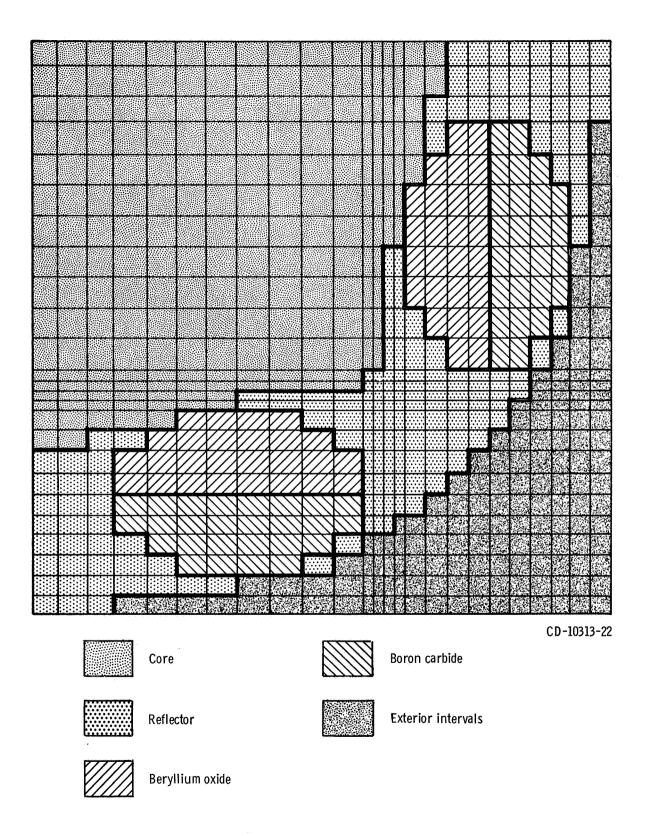


Figure 1. - Test case configuration.

The configuration used for testing these modifications is shown in figure 1. It is a rectangular coordinate representation of the transverse section of a cylindrical reactor. The reactor is fueled with uranium nitride enriched in the uranium-233 isotope ($\rm U^{233}N$) and uses lithium-7 ($\rm Li^7$) as a coolant. Control is effected by the rotation of noncentral drums containing boron carbide ($\rm B_4C$) and the reflector is beryllium oxide (BeO).

Eight group cross sections, seven fast and one thermal, generated from the GAM-II (ref. 8) and GATHER-II (ref. 9) library are used. While this configuration was run to verify the accuracy of all the modifications, the angular quadrature results are based primarily on a one-dimensional representation of this core using two-dimensional quadrature sets.

ANGULAR QUADRATURE MODIFICATIONS

Analysis

Examination of the flux values established during the early iterations of a high-order angular quadrature calculation indicates that a large number of unnecessary numerical steps are performed in establishing an accurate preliminary scalar flux distribution. The use of any of the previously described methods (refs. 5 to 7) should be a valid, but perhaps inefficient, procedure for establishing preliminary scalar flux distribution. The basic question of the optimum manner in which to approach the final solution requires a more general modification of the standard \mathbf{S}_n coding. Options should be included which would allow studies to be made of the effect on convergence of using any progression of quadratures in conjunction with arbitrary termination criteria. In addition, since most reactor configurations involve energy dependent cross sections in which the optimum quadrature order would not be identical for all energy groups, it would be of interest to observe the effect of permitting the quadrature order to be a function of the energy.

Since the lower order quadratures cannot be expected to yield scalar flux distributions with an accuracy equivalent to that of higher order quadratures, there is a little point in solving the lower order calculation to the same degree of convergence required for the final calculation. The major benefit in the final calculation should be derived from the use of a trial scalar flux which minimizes the number of inner iterations required for convergence on the final quadrature and not from fully converged low-order scalar fluxes. An important question in this regard is that of determining the optimum point at which to effect the quadrature variations.

In order to study the effect on solution time of the modifications discussed, the computer program previously referenced (ref. 3) has been altered to perform the following sequences of operation:

- (1) Any number of preliminary lower order quadrature sets may be used.
- (2) The use of a given quadrature set may be terminated either by completion of a given number of outer iterations or by attaining to some specified degree of convergence.
- (3) When the number of outer iterations is specified, a convergence criterion may be used which will terminate the calculation if convergence on that set is attained before all the outers are performed.
- (4) The final quadrature order may be made a function of the energy group. This feature may be used with or without the preliminary lower order calculation.

Sequences (2) and (3) imply that more than one degree of convergence may be used on the same quadrature set. This, in effect, serves to limit the number of inner iterations in the initial phases of the calculation. The multiple sets of direction numbers need not be read in as the program generates moment modified sets (ref. 10) as required. In addition, all the options available in the original code, including convergence tests and acceleration procedures, are retained. None of the modifications made which involve varying the angular quadrature order during the course of the calculation should affect the accuracy of the final results. Convergence on the final values of the angular fluxes, eigenvalues, and other quantities must not depend on the manner in which the calculation is begun. This is also true, within the framework of the quadrature orders used, for the modification in which quadrature is made a function of the energy. The main problem here is in not having a foreknowledge of the quadrature required to represent a given energy group accurately.

RESULTS

The most important consideration concerning the use of preliminary low-order quadratures is that of determining the optimum manner in which to approach final convergence. Results from the one-dimensional cases collected in table I indicate that this optimum method depends on the order of the final quadrature desired.

The terminology in table I is best explained by example. In case 1a, the quadrature sequence S_2 , S_8 and the criterion sequence 2I, 10^{-4} mean that the problem was started as S_2 and after two outer iterations 2I, it was switched to an S_8 calculation and completed with a convergence criterion of 10^{-4} . Note that the last value in the quadrature sequence and in the criterion sequence are the same as for the base case.

Although the running times for the problems of table I are dependent, to some extent, on both the particular computer and \mathbf{S}_n program used, the test case results allow some general conclusions to be drawn.

The strategy used to effect maximum time reduction depends on the order of the final quadrature desired. For the test case, with an S_8 final quadrature, the optimum ap-

TABLE I. - QUADRATURE MODIFICATIONS

(a) Various strategies used for convergence of an S₈ problem (eigenvalue = 1,6051 for all cases)

Case 1	Quadrature sequence	Criterion sequence ^a	Running time, min
Base a b c d e f g h	S ₈ S ₂ , S ₈ , S ₈ S ₂ , S ₄ , S ₈	10 ⁻⁴ 2I, 10 ⁻⁴ 3I, 10 ⁻⁴ 10 ⁻² , 10 ⁻⁴ 10 ⁻³ , 10 ⁻⁴ 10 ⁻⁴ , 10 ⁻⁴ 2I, 10 ⁻² , 10 ⁻⁴ 2I, 10 ⁻³ , 10 ⁻⁴ 2I, 10 ⁻³ , 10 ⁻⁴ 2I, 10 ⁻³ , 10 ⁻⁴	2. 53 1. 90 1. 84 1. 63 1. 77 2. 0 1. 52 1. 36 1. 70

(b) Various strategies used for convergence of above problem to S_{16} (eigenvalue = 1.0052 for all cases)

Case 2	Quadrature sequence	Criterion sequence ^a	Running time, min
Base	S ₁₆	10 ⁻⁴ 2I, 4I, 10 ⁻³ , 10 ⁻⁴ 4I, 10 ⁻³ , 10 ⁻⁴ 10 ⁻⁴ , 10 ⁻⁴ , 10 ⁻⁴	9. 33
a	S ₂ , S ₄ , S ₈ , S ₁₆		3. 98
b	S ₂ , S ₁₆ , S ₁₆		4. 80
c	S ₂ , S ₄ , S ₈ , S ₁₆ , 10 ⁻⁴		5. 50

^aThe number of outer iterations I run on the indicated quadrature set is represented by nI.

proach was to use only a single preliminary quadrature. This is best illustrated by comparing case 1g, which used only an S_2 start, with case 1h, which used both an S_2 and an S_4 preliminary calculation, and whose running time to final convergence was longer. For the same test case with an S_{16} final quadrature, best results were obtained with the use of multiple preliminary quadratures. As an example, case 2a, which employed three preliminary quadrature orders, converged much more rapidly than case 2b, which used only the S_2 preliminary calculation. In general, it appears that calculations involving low-order final quadratures are best accomplished with a single intermediate quadrature while high-order calculations require the use of multiple preliminary quadrature sets.

For those problems in which the use of only a single preliminary quadrature is most efficient, a number of trial cases (1a to 1g) where run in order to determine when to shift from the preliminary to the final quadrature. As discussed previously, full convergence on the preliminary quadrature is probably not desirable. This is borne out by case 1e

which converged the S_2 start to the final 10^{-4} criterion and required more running time than any of the other methods applied. These cases also indicate that final convergence is best approached by first performing several outer iterations and then converging to some intermediate criterion on the final quadrature. The use of this intermediate criterion essentially acts to limit the number of inner iterations per outer iteration during that portion of the calculation when the flux distribution is changing rapidly. The same effect could be achieved by directly controlling the number of inner iterations per outer iteration but this procedure affords no way of ensuring that the flux in each energy group is equally well converged.

For those problems in which multiple quadratures are used to approach final convergence, it is more difficult to specify an optimum approach. The calculation of all of the large number of permutations afforded by allowing both a given number of outer iterations and an intermediate convergence for each quadrature criterion would require an inordinate amount of machine time. Again, however, case 2c demonstrates that running to full convergence on each preliminary quadrature is less efficient than use of other available options. Consideration of the results of the cases run shows that the shortest running time for the S_{16} solution was achieved by performing a limited number of outer iterations on both an S_2 and an S_4 preliminary calculation followed by intermediate convergence on an S_8 quadrature and, finally, by final convergence on the S_{16} solution. Case 2a, which followed this pattern, reduced the time required to obtain an S_{16} result by more than 50 percent.

The program modification which allows the quadrature order to be specified by energy group was also tested on the same base case but with the quadrature sets for the eight energy groups arbitrarily chosen as $2S_8$, $4S_4$, and $2S_2$ starting with the highest energy group. For this test case the running time was reduced by about 60 percent. The low-order quadrature start may also be used in conjunction with this modification to reduce the running time further. The value of this modification is questionable due to the difficulty involved in specifying appropriate quadrature orders.

SPATIAL QUADRATURE MODIFICATIONS

Analysis

Present applications of the discrete ordinates method require that a continuous spatial mesh be employed. This means that the interval spacing used in one direction must be retained over the whole configuration. For example, the use of rectangular coordinates to represent the cylindrical boundary shown in figure 1 requires retention of the extraneous intervals lying outside the configuration. The typical reactor problem also

contains larger homogeneous regions which should not require the same detailed spatial treatment as is necessary near material interfaces or boundaries. Since the angular flux in each discrete direction must be repetitively computed for each mesh interval, reduction or elimination of unnecessary intervals would improve the efficiency of the calculation. Another desirable option would be to obtain an initial improved flux estimate by first solving a less detailed problem.

Although consideration of the constant spatial quadrature requirement indicates many possible modifications, those accomplished for this study were restricted to the following:

- (1) An option for specifying the number of mesh intervals in the configuration in one direction as a function of the other direction is added. In effect, this allows the normal mesh spacing to be retained but permits the truncation of individual rows in the configuration, as shown in figure 2. The boundary conditions are then applied to the initial and final remaining intervals in each row.
- (2) An option for varying the mesh interval spacing in the interior regions for both directions is developed. In effect, this allows several intervals to be combined into one and permits the angular fluxes to be calculated only once, in each inner iteration, for this larger interval rather than once for each original separate interval. This option is depicted in figure 3.
- (3) If solution accuracy equivalent to that of the original \mathbf{S}_n mesh is required, a provision is made for expanding the scalar flux distribution developed in part (2) and performing final iterations on the original mesh configuration.

Because of the numerous ways in which alterations to the spatial mesh portion of the standard \mathbf{S}_n flow may be accomplished, no spatial modification may be regarded as unique since the same end effect, the reduction of the number of intervals to be treated in the calculation, may be achieved using many different approaches. In general, the modifications described here have been restricted to Cartesian coordinates and an attempt made to keep the additional input as simple as possible.

Results

The first modification tested was that in which the number of intervals in each row is allowed to vary. This option is primarily useful where it is necessary to use rectangular coordinates to analyze a cylindrical core such as shown in figure 2. Any combination of the normal boundary conditions is permitted so that the quarter, half, or full configuration may be run. In the standard S_n treatment, it is necessary to run the complete rectangular mesh with some artificial material in the extraneous intervals. It is possible to compare the accuracy of this modification with that of the standard treatment by inserting a "perfect absorber" into these intervals. Comparison of the eigenvalues from such

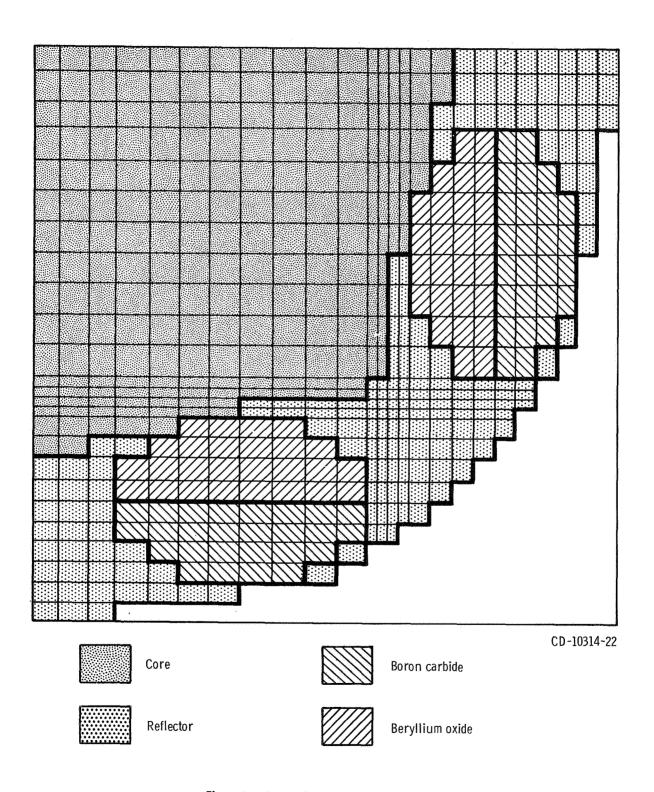


Figure 2. - Interval truncation modification.

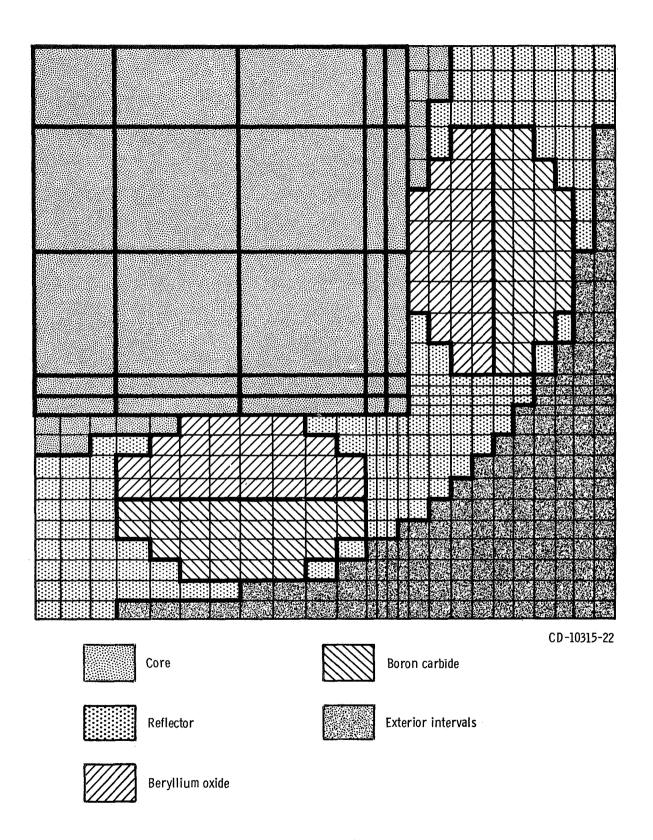


Figure 3. - Interval combination modification.

calculations shows agreement, at the end of each outer iteration, to better than the accuracy required by the convergence criterion used. The time reduction depends, of course, on the complexity of the original case and on the number of intervals deleted. For the configuration of figure 2, with the exterior intervals removed from the computation, the time reduction is approximately 25 percent.

As a test of the leakage calculation, a simple case was run using cylindrical coordinates in the original code to obtain the eigenvalue and leakage for a 10-centimeter-radius cylinder with no internal details. This run was then compared with the interval deletion modification results using a 10-interval approximation of the cylindrical boundary. The comparison yields

	Method	Eigenvalue	Leakage per
	:		source
,			neutron
	Original TDSN	0.9623	0.0377
	Interval deletion	.9617	. 0383

which is quite accurate since only 10 steps were used to approximate the boundary.

The second modification, in which interior mesh intervals within homogeneous regions of the core are combined, is the most complex in terms of alterations made to the standard flow. Since the method of implementing any such scheme is quite arbitrary, a brief description of the procedure followed is given.

The normal spatial mesh is first defined. Two interior coordinate boundaries are then specified. Within these boundaries, the interval reduction, or combination, may be applied. Each original region is comprised of a given number of intervals, bounded by mesh lines. The interval reduction is accomplished by choosing the number of mesh lines, in each direction, to be eliminated. Thus, sets of from one to the total number of interval lines may be removed. As an example, if sets of two are removed, two interval boundaries are deleted, the next is retained, the next two removed, and the process continued until the outer region boundary is reached. The elimination is performed independently in each coordinate direction with the only restriction being that the last remaining interval boundaries must coincide with the original region boundaries. Figure 3 indicates the results of applying this process to the test case. Since the process results in dissimilarly sized adjacent intervals, some assumption is necessary concerning the behavior of the angular fluxes across such boundaries. No attempt has been made in this study to develop interpolation formulas for such cases and simple flux averages have been used to extrapolate the angular fluxes.

As an example of the use of this modification, the configuration shown in figure 3 was run with the intervals combined as indicated. This problem should represent an extreme test of the modification since some intervals have been combined in regions, such as near the control drums and material interfaces, where the angular fluxes are expected to vary rapidly. Two test cases were run and compared with the results of the original version of the program in order to compare both eigenvalues and reactivities. The second case is also as in figure 3 but with the control drums rotated 90° clockwise. Results for the first case are

Method	Time, min	Eigenvalue
Original TDSN Interval reduction	22.88 15.44	

The eigenvalues differ by 0.39 percent. The running time is reduced by about 35 percent. For the 90° control drum rotation, the results are

Method	Time, min	Eigenvalue
Original TDSN Interval reduction	17. 22 11. 96	1.285 1.280

The eigenvalues differ by 0.32 percent with a time reduction of about 33 percent. A comparison of the control reactivities shows that the original version yields 2.28 percent $\delta k/\bar{k}$ and the interval reduction scheme 2.21 percent $\delta k/\bar{k}$. This is good agreement in view of the fact that intervals have been deleted in regions where the flux does not conform to an assumption of relative constancy.

The most general application of this modification is to generate a preliminary scalar flux guess for use in a final calculation over the original spatial mesh. To demonstrate this, a configuration similar to that shown in figure 3 was run, using a coarse spatial mesh with less detail in the control drum region, for three outer iterations of the reduced mesh. The scalar fluxes resulting from this calculation were then expanded to fit the original mesh, and the final iterations converged on this mesh. A comparison of the times involved yields

Method	Time, min	Eigenvalue
Original TDSN	13.32	1. 145
Coarse mesh Original mesh	4. 192 +3. 830	1. 135 1. 145
Total time	8, 022	

for a time reduction of approximately 40 percent.

CONCLUSIONS

Some general conclusions regarding the utility of modifications of the type accomplished for this study may be drawn as a result of the test cases run. These conclusions depend, to some extent, on the accuracy required for the final calculation.

For repetitive survey calculations, in which high accuracy is not required, the use of approximate solutions can greatly reduce machine running times. For the same computer time, the results are more accurate than obtained with a straight S_n calculation. For the modification using a less detailed angular representation in the preliminary calculations, an approximate solution may be obtained by permitting the quadrature order to be a function of the energy group. While the question of the quadrature order required to describe a given energy group adequately may be difficult, test case results have not varied greatly with reductions in quadrature order. Moreover, the energy dependent quadrature solutions, particularly when combined with a low-order preliminary calculation, afford a means of rapidly obtaining approximate answers. For the modification in which interval boundaries are omitted, an approximate solution is obtained by combining less important mesh intervals. The question of which intervals to combine is much less difficult than that of predetermining angular quadrature orders. Since the configuration to be analyzed is known and the spatial angular flux averages postulate a slowly varying angular flux, intervals should be combined only in regions which are homogeneous and removed from material interfaces. The test case results, in which the interval reduction scheme was applied to regions which do not rigorously satisfy the postulate, indicate that this limitation is not severe.

From those sample problems in which converged solution accuracy identical to that of the standard \mathbf{S}_n method application was required, several conclusions may be drawn:

1. If more than one angular quadrature set is employed, requiring full convergence on the preliminary sets significantly increases running time.

- 2. For problems specifying lower order final angular quadratures ($\leq S_8$), the most efficient approach to final convergence is through the use of a single preliminary S_2 quadrature followed by partial convergence on the final quadrature. The partial convergence limits the number of inner iterations and assures that the fluxes are equally well converged in each group before entering the final calculation.
- 3. For problems requiring high-order final angular quadratures (>S₈) the greatest time reduction is observed when several intermediate quadrature sets are used successively to approach final convergence.
- 4. For problems requiring highly detailed spatial information, the time to final convergence is reduced when a relatively coarse mesh is used to represent the spatial and material configuration in the preliminary calculation.

It may be concluded that modifications of the type outlined are capable of significantly reducing machine execution times without impairing solution accuracy.

Lewis Research Center,

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REFERENCES

- 1. Carlson, Bengt G.: Solution of the Transport Equation by $\, {\rm S}_n \,$ Approximations. Rep. LA-1891, Los Alamos Scientific Lab., Feb. 1955.
- 2. Lathrop, K. D.: DTF-IV A Fortran-IV Program for Solving the Multigroup Transport Equation with Anisotropic Scattering. Rep. LA-3373, Los Alamos Scientific Lab., July 1965.
- 3. Barber, Clayton E.: A Fortran IV Two-Dimensional Discrete Angular Segmentation Transport Program. NASA TN D-3573, 1966.
- 4. Mynatt, F. R.: DOT, A Two-Dimensional Discrete Ordinates Transport Code. Rep. K-1694, Union Carbide Corp., 1967.
- 5. Carlson, B.; Worlton, W. J.; Gruber, W.; and Shapiro, M.: DTF Users Manual. Rep. UNC Phys/Math-3321, United Nuclear Corp., Nov. 1963.
- 6. Carlson, B.; Lee, C.; and Worlton, J.: The DSN and TDC Neutron Transport Codes. Rep. LAMS-2346, Los Alamos Scientific Lab., Oct. 1959.

- 7. Alexander, J. H.; Hinman, G. W.; and Triplett, J. P.: GAPLSN A Modified DSN Program for the Solution of the One-Dimensional Anisotropic Transport Equation. Rep. GA-4972, General Dynamics Corp., Mar. 1964.
- 8. Joanou, G. D.; and Dudek, J. S.: GAM-II. A B₃ Code for the Calculation of Fast-Neutron Spectra and Associated Multigroup Constants. Rep. GA-4265, General Dynamics Corp., Sept. 16, 1963.
- 9. Joanou, G. D.; Smith, C. V.; and Vieweg, H. A.: GATHER-II. An IBM-7090 Fortran-II Program for the Computation of Thermal-Neutron Spectra and Associated Multigroup Cross Sections. Rep. GA-4132, General Dynamics Corp., July 8, 1963.
- 10. Carlson, B. G.; and Bell, G. I.: Solution of the Transport Equation by the S_n Method. Nuclear Data and Reactor Theory. Vol. 16 of Proceedings of the Second United Nations International Conference on the Peaceful Uses of Atomic Energy. United Nations, 1968, pp. 535-549.

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-National Aeronautics and Space Act of 1958

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